



Oscillator Strengths and Integral Cross Sections of the Valence-shell Excitations of Acetylene Studied by the High-energy Electron-scattering

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Abstract

The oscillator strengths and integral cross sections of the valence-shell excitations of acetylene have significant applications in the studies of interstellar gases. In the present work, the generalized oscillator strengths (GOSs) of the valence-shell excitations of acetylene have been determined by the fast-electron-scattering technique at an incident electron energy of 1500 eV and an energy resolution of 70 meV. The optical oscillator strengths (OOSs) of the valence-shell excitations of acetylene have been obtained by extrapolating the GOSs to the limit of the squared momentum transfer $K^2 \rightarrow 0$. The present OOSs give an independent cross-check to the previous experimental and theoretical results, and the discrepancies between the present OOSs and the photoabsorption ones are analyzed in detail for the R30–R33 excitations. The integral cross sections of the valence-shell excitations of acetylene have been obtained systematically from the threshold to 5000 eV for the first time with the aid of the newly developed *BE*-scaling method. The present OOSs and integral cross sections of the valence-shell excitations of acetylene are the basic data for the astrophysical study and are conducive to deepening our understanding of the atmospheres of Jupiter and Saturn, and other outer planets and satellites.

Key words: methods: laboratory; molecular – molecular data

1. Introduction

As an important astrophysical molecule, acetylene is abundant in the interstellar medium (Prasad & Huntress 1980), carbon stars (Ridgway et al. 1976; Jorgensen & Johnson 1991), and planetary atmospheres (Mitchell et al. 1981; Shemansky et al. 2005). It is well known that spectrum observation is effective for the identification and determination of abundances of hydrocarbon species in space, and spectrum observation is one of the most important missions for many spacecraft, such as *Voyager* and the *Cassini* Ultraviolet Imaging Spectrograph (Broadfoot et al. 1981; Sandel et al. 1982; Smith et al. 2007; Shemansky & Liu 2012; Koskinen et al. 2013; Vervack & Moses 2015). Coincidentally, acetylene is one of the strongest absorbers in the vacuum ultraviolet (VUV) region for astronomical observations and is thus a key diagnostic in investigations of giant planets (Wagener et al. 1985). For example, the distinctive features of the VUV spectrum of acetylene were first detected in Saturn with the *International Ultraviolet Explorer* (*IUE*) by Moos & Clarke (1979), then, from *IUE* observations of Saturn (Chen et al. 1991) it was clearly confirmed that acetylene is the dominant absorber. In addition to serving as an important research object, Titan was investigated by many spacecraft, such as *Voyager 1* and 2 in the 1980s (Broadfoot et al. 1981; Sandel et al. 1982; Vervack & Moses 2015) and *Cassini* more recently (Smith et al. 2007; Shemansky & Liu 2012; Koskinen et al. 2013). During the Titan flyby on 2004 December 13, the absorption spectra of Titan's atmosphere were recorded by *Cassini*; these are the basic and key data for determining the compositions of Titan's atmosphere (Shemansky et al. 2005). In order to explain these complex spectra, the optical oscillator strengths (OOSs) and integral cross sections (ICSs) of the acetylene molecule are the basic input parameters for the theoretical models (Cheng et al. 2011). Moreover, according to a series of photochemical models (Campbell

et al. 2012; Campbell & Brunger 2013), with the aid of the OOSs and ICSs of acetylene and other hydrocarbon molecules, the abundance of atmospheric constituents, the atmospheric motions, and seasonal variations of Titan's atmosphere with the variation of the external environment (Campbell & Brunger 2013) can be obtained. Additionally, the OOSs of acetylene have been employed widely in the models of the atmospheres of Jupiter, Saturn, Uranus, Neptune, and Triton (Wu et al. 2001). So quantitative dynamic parameters for the valence-shell excitations of acetylene are needed to understand many astrophysical and photochemical processes.

With such high importance and various applications, the OOSs of the valence-shell excitations of acetylene have received much attention. Since the original observation of the discrete VUV photoabsorption spectrum of acetylene by Price (1935), the acetylene molecule has been investigated extensively both experimentally and theoretically. Herzberg (1966) and Robin (1985) summarized and reviewed the works reported before 1985, but a quantitative measurement of the photoabsorption cross sections of acetylene was reported only once (Nakayama & Watanabe 1964). Since then, the OOSs of the valence-shell excitations of acetylene were measured by Suto & Lee (1984) with an energy resolution of 0.04 nm, by Smith et al. (1991) with an energy resolution of better than 0.005 nm, by Wu et al. (2001) with an energy resolution of 0.007 nm, and by Cheng et al. (2011) with an energy resolution of 0.02 nm via the photoabsorption method. In principle, the photoabsorption measurements provide a direct determination of the OOSs of atoms and molecules; however, the insufficient instrumental resolution may result in the line-saturation effect and complicate the analysis of strong absorption lines. This line-saturation effect is particularly likely to occur when making photoabsorption measurements on intense, narrow, discrete excitations using the Beer–Lambert law. When the

electron-scattering technique is operated at a negligibly small momentum transfer, it can be used to simulate the photoabsorption process and determine the OOSs of atoms and molecules; this is called the dipole (e, e) method. Compared with the photoabsorption method, the dipole (e, e) method has the remarkable advantage of being free from the line-saturation effect, due to its nonresonant excitation character, though its typical energy resolution of tens of meV is much lower than that of the photoabsorption method. Using the dipole (e, e) method, Cooper et al. (1995) reported the OOSs of the valence-shell excitations of acetylene. Although the OOSs of the valence-shell excitations of acetylene have been reported widely using the photoabsorption method and the dipole (e, e) method, significant discrepancies and arguments persist for these previous results (Cooper et al. 1995; Cheng et al. 2011). Under these circumstances, it is very important to investigate the OOSs of the valence-shell excitations of acetylene with a further experiment that can provide an independent cross-check on the previous results.

The ICSs of the valence-shell excitations of acetylene have not been reported until now, to the best of our knowledge. It is well known that ICSs can be determined by integrating the corresponding differential cross sections (DCSs) of the atoms and molecules from 0° to 180° measured by the electron-scattering. However, only some electron-energy-loss spectra were obtained in previous works (Lassette et al. 1968; Stradling 1977; Wilden et al. 1980; Brunger et al. 1990), and no absolute DCSs for the valence-shell excitations of acetylene were reported.

Following the discussion above, it is very significant and important to investigate the OOSs and ICSs of the valence-shell excitations of acetylene with additional experiments that can provide an independent cross-check on the previous OOSs, and provide the systematic ICSs of the valence-shell excitations of acetylene. In the present work, the generalized oscillator strengths (GOSs) of the valence-shell excitations of acetylene have been determined by the high-energy electron-scattering technique at an incident electron energy of 1500 eV and an energy resolution of 70 meV. Additionally, the OOSs of acetylene have been obtained by extrapolating the GOSs to the limit of the squared momentum transfer $K^2 \rightarrow 0$, and the ICSs of the valence-shell excitations of acetylene have been obtained systematically from the threshold to 5000 eV for the first time with the aid of the *BE*-scaling method. For clarity, the vibronic states are represented by their term names and principal and vibrational quantum numbers such that $R' n = 3, \nu'_2 = 1$; they are written as R'31 in this paper.

2. Experimental Method

In this work, the GOSs of the valence-shell excitations of acetylene have been determined by a high-resolution fast-electron-energy-loss spectrometer, which is described in detail in our previous works (Wu et al. 1995; Xu et al. 1996; Liu et al. 2001). Briefly, the spectrometer consists of an electron gun, a hemispherical electrostatic monochromator made of aluminum, a rotatable energy analyzer of the same type, an interaction chamber, a number of cylindrical electrostatic optics lens, and a position sensitive detector based on the micro-channel plates for detecting the scattered electrons. All of these components are enclosed in three separate stainless steel chambers. For this experiment, the spectrometer was operated

at an incident electron energy of 1500 eV and an energy resolution of about 70 meV.

In order to simplify the normalization process and improve the accuracy of the experimental results, the standard relative flow technique (Khakoo & Trajmar 1986; Nickel et al. 1989; Liu et al. 2017; Ni et al. 2017) was used in this experiment. First, mixed gases of helium and acetylene with respectively controlled flowed rates flowed into the interaction chamber simultaneously and continuously. Then, the intensity ratios of the excited states of the sample acetylene to the referenced standard transition (here the $1s^{21}S_0 \rightarrow 1s2p^1P_1$ of helium) were determined from the measured energy-loss spectra. Finally, with these ratios we could determine the GOSs of acetylene by normalizing them to the GOS of the $1s^{21}S_0 \rightarrow 1s2p^1P_1$ transition of helium (Xu et al. 1996; Cann & Thakkar 2002; Han & Li 2006), which has been measured and calculated with a high accuracy. The normalization processes can be found in detail in Liu et al. (2017) and Ni et al. (2017).

According to the Bethe theory (Bethe 1930, 1932; Inokuti 1971; Bransden & Joachain 2003), the DCS for a definite excitation in the high-energy electron-scattering can be factorized into two factors: one dealing with the incident electron only, the other, referred to as the GOS, dealing with the target only. The GOS is defined as:

$$f(\mathbf{K}, E_n) = \frac{E_n p_0}{2 p_a} K^2 \frac{d\sigma_n}{d\Omega} = \frac{2E_n}{K^2} \left| \langle \Psi_n | \sum_{j=1}^N \exp(i\mathbf{K} \cdot \mathbf{r}_j) | \Psi_0 \rangle \right|^2. \quad (1)$$

Here $f(\mathbf{K}, E_n)$ and $d\sigma_n/d\Omega$ stand for GOS and DCS, while Ψ_0 and Ψ_n are the N -electron wavefunctions for the initial and final states, respectively. E_n and $\mathbf{K}$ are the excitation energy and momentum transfer, while p_0 and p_a are the incident and scattered electron momenta, respectively. $\mathbf{r}_j$ is the position vector of the j th electron.

In the measurement procedures, the background pressure in the vacuum chamber was 5×10^{-5} Pa, and the flows of helium and acetylene were set as 0.5 sccm and 0.3 sccm, respectively, and were controlled by the CS200 mass flow meters produced by the Beijing Sevenstar Electronic Co. Ltd with a declared accuracy of better than 2%. The true zero angle was calibrated by the symmetry of the angular distribution of the inelastic scattering signals of the $1s^{21}S_0 \rightarrow 1s2p^1P_1$ peak of helium around the geometry nominal 0° . To exclude the influence of the pressure effect from the multiple-scattering (Zhong et al. 1997), the electron-energy-loss spectra were recorded with different flows at some angles. The GOSs of the valence-shell excitations of acetylene at different pressures are in coincidence within the experimental uncertainties, which indicates that the present work is free from the pressure effect.

The typical electron-energy-loss spectrum of acetylene at a scattering angle of 3° is shown in Figure 1(a), and a 2D map for the GOS densities (GOSDs) of the valence-shell excitations of molecular acetylene versus the energy-loss and squared momentum transfer measured is shown in Figure 1(b), in which the 2D of the valence-shell excitations of acetylene was obtained by transferring the measured electron-energy-loss spectra to the GOSD scale at every scattering angle. In Figure 1(a), the assignments for the valence-shell excitations of acetylene were taken from Suto & Lee (1984). In the 8.0–8.9 eV region, the intensities for the individual transitions of R30–R33 were obtained by numerically integrating the

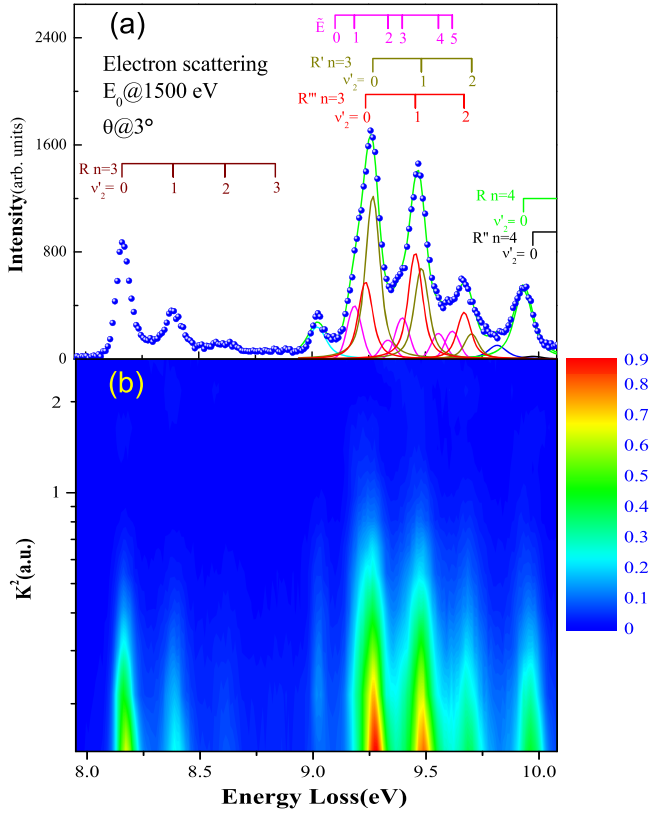


Figure 1. (a): A typical electron-energy-loss spectrum of the valence-shell excitations of acetylene at an incident electron energy of 1500 eV and a scattering angle of 3° . The solid lines are the fitted curves. (b): 2D map of the GOSDs of molecular acetylene vs. the energy-loss and squared momentum transfer measured by the present high-energy electron-scattering.

spectra under the peak in the ranges of 8.00–8.28 eV, 8.28–8.51 eV, 8.51–8.74 eV, and 8.74–8.90 eV, respectively, and a similar treatment has been used to determine the OOSs of the R30–R33 transitions by Cooper et al. (1995). In the 8.9–10.0 eV region, the least-squares fitting method was used to fit the experimental spectra by the Gaussian curve in order to determine the intensities of the valence-shell excitations. Note that the present energy resolution of 70 meV is insufficient for separating the excitations from the curve-fitting procedures, so the GOSs for the sum of the excitations, i.e., $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$, are given.

Unlike the Rydberg series of acetylene, the virtual valence $\tilde{E}$ state is not linear and has the v_4 and v_5 vibrations, which are the *trans* and *cis* bending vibrational modes, respectively. The vibronic transitions of the $\tilde{E}$ state located at 9.102, 9.187, 9.335, 9.398, 9.558, and 9.619 eV, as used by Cooper et al. (1995), are written as $\tilde{E}0$ – $\tilde{E}5$ in the present work for clarification. According to the assignment of Suto & Lee (1984), the transitions of the $\tilde{E}0$, $\tilde{E}1$, $\tilde{E}2$, and $\tilde{E}4$ each only include one vibronic transition, while the transitions of $\tilde{E}3$ and $\tilde{E}5$ each include two vibronic transitions due to the narrow energy interval (about 30 meV) between them.

The present GOSs of the valence-shell excitations of acetylene are shown in the corresponding figures and Table 1. The experimental errors of the GOSs in the present work are from the definite angular resolution, the statistical counts, the fitting procedure, and the normalizing procedure, which are also shown in the corresponding figures and Table 1.

3. Results and Discussion

According to Lassette (1965) and Tanaka et al. (2016), the GOSs of the valence-shell excitations of atoms and molecules can be fitted by the formula

$$f(\mathbf{K}, E_n) = \frac{x^M}{(1+x)^{(l+l'+M+5)}} \sum_{m=0}^{\infty} \frac{f_m x^m}{(1+x)^m}. \quad (2)$$

Here, $x = K^2/\alpha^2$ with $\alpha = (2I)^{1/2} + [2(I - E_n)]^{1/2}$, and I is the ionization energy. l and l' are the orbital angular momenta of the initial and final states of the excited electron, while M is an integer that is relevant to the transition multipolarity, and f_m are the fitting parameters. Since the ionization energy I of an electron in a molecule is defined only in the context of a simply independent particle model by Lassette (1965), it is better to simply take α^2 as a fitting parameter along with f_m , as proposed by Kim (2007).

The present GOSs of the R30, R31, R32, and R33 excitations of acetylene are shown in Figure 2. It is clear from Figure 2 that the GOSs from the intense R30 excitation to the weak R33 excitation have similar tendencies, and the positions of the minima of the GOSs are at about 1.0 au. Meanwhile, the present GOSs of the $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ excitations of the acetylene molecule, and their fitted curves, have been obtained and are shown in Figure 3. There are no other theoretical calculations and experimental measurements available for comparison, to the best of our knowledge.

According to Equation (2), the OOSs f_0 of the dipole-allowed transitions of acetylene molecule can be obtained by extrapolating the GOSs to the limit of the squared momentum transfer $K^2 \rightarrow 0$. The present OOSs of the R30, R31, R32, and R33 excitations of acetylene are shown in Figure 4 and Table 2 along with the previously available ones from the dipole (e, e) measurement method (Cooper et al. 1995; see Figure 4(a)), the photoabsorption measurements (Moe & Duncan 1952; Gedanken & Schnepf 1976; Suto & Lee 1984; Smith et al. 1991; Wu et al. 2001; Cheng et al. 2011) (see Figure 4(b)), and the theoretical calculations (Demoulin & Jungen 1974; Jensen et al. 1990) (see Figure 4(c)). As shown in Figure 4(a), the present OOSs of the R30, R31, and R32 transitions match the dipole (e, e) ones of Cooper et al. (1995) very well. As for the weakest R33 transition, the difference between the present result and the dipole (e, e) result of Cooper et al. (1995) may be from the extrapolating process or the influence of the strong transitions.

The previous OOSs of the R30, R31, R32, and R33 excitations of acetylene measured by the photoabsorption method (Moe & Duncan 1952; Gedanken & Schnepf 1976; Suto & Lee 1984; Smith et al. 1991; Wu et al. 2001; Cheng et al. 2011) are also shown in Figure 4(b). It can be seen that the early photoabsorption results of Gedanken & Schnepf (1976) and Moe & Duncan (1952) are obviously lower than the present OOSs, which may be due to the limitations of the technique at that time. Additionally, it is also clear from Figure 4(b) that the present OOS of the R30 transition is consistent with that of Smith et al. (1991) at an energy resolution of better than 0.005 nm, and is only slightly higher than the photoabsorption results of Wu et al. (2001) at the energy resolution of 0.007 nm, and the results of Cheng et al. (2011) at the energy resolution of 0.02 nm and Suto & Lee (1984) at the energy resolution of 0.04 nm. To

Table 1
The Present GOSs of the Valence-shell Excitations of Acetylene

K^2 (au)	R30	R31	R32	R33	$\tilde{E}0 + \tilde{E}1 + \tilde{E}2$ +R'30 + R''30	$\tilde{E}3 + \tilde{E}4 + \tilde{E}5$ +R'31 + R''31	R'32 + R''32	R40 + R''40
0.14	55.30(3.34)	31.30(3.43)	11.02(2.65)	5.81(1.25)	109.88(6.00)	124.02(7.46)	34.07(2.34)	44.97(2.73)
0.21	36.19(2.30)	21.10(1.82)	8.36(0.58)	5.06(1.46)	87.43(4.76)	94.39(5.85)	24.25(1.98)	30.86(1.95)
0.31	20.78(1.69)	13.51(3.80)	5.61(2.67)	3.21(1.31)	68.34(4.38)	67.57(4.30)	16.88(1.35)	19.26(1.29)
0.41	11.99(1.11)	7.68(2.55)	3.62(1.73)	2.09(0.92)	49.14(3.43)	48.01(3.35)	11.90(1.11)	12.13(0.82)
0.54	5.81(0.72)	3.93(2.08)	2.25(1.49)	1.40(0.39)	34.26(2.33)	32.93(2.30)	8.22(0.83)	7.43(0.55)
0.66	3.52(0.41)	2.54(0.22)	1.46(0.17)	0.98(0.46)	26.54(1.74)	24.37(1.67)	5.93(0.60)	5.26(0.42)
0.81	1.62(0.89)	1.16(0.54)	0.78(0.27)	0.56(0.37)	16.66(1.12)	14.78(1.08)	3.89(0.45)	2.98(0.30)
0.98	1.15(0.34)	0.99(0.13)	0.65(0.09)	0.49(0.22)	11.16(0.83)	10.32(0.85)	2.42(0.34)	2.23(0.23)
1.19	1.39(0.44)	1.17(0.15)	0.70(0.12)	0.37(0.23)	7.07(0.61)	6.63(0.63)	1.45(0.31)	1.86(0.26)
1.39	1.74(0.36)	1.35(0.14)	0.72(0.10)	0.34(0.22)	5.40(0.44)	4.70(0.44)	1.23(0.23)	1.71(0.23)
1.64	2.28(0.36)	1.78(0.13)	0.93(0.10)	0.49(0.16)	4.51(0.78)	4.33(0.69)	0.80(0.36)	2.23(0.41)
2.18	2.29(0.31)	1.97(0.13)	1.12(0.09)	0.48(0.17)	3.95(0.54)	3.53(0.72)	0.74(0.43)	2.02(0.16)
2.76	2.11(0.57)	1.75(0.20)	0.96(0.12)	0.53(0.22)	4.10(0.41)	3.30(0.95)	0.79(0.64)	1.80(0.21)

Note. The listed data are amplified by a factor of 10^3 . The data in parentheses represent the corresponding experimental uncertainties.

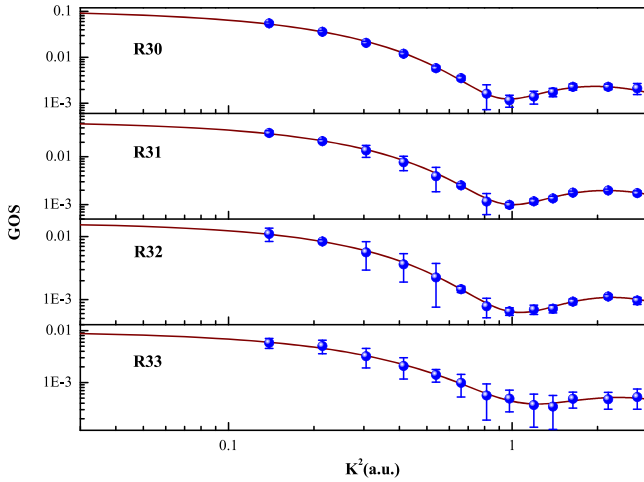


Figure 2. Present GOSs of the R30, R31, R32, and R33 excitations of the acetylene molecule. The dots are the present results, and the solid lines are their fitted curves.

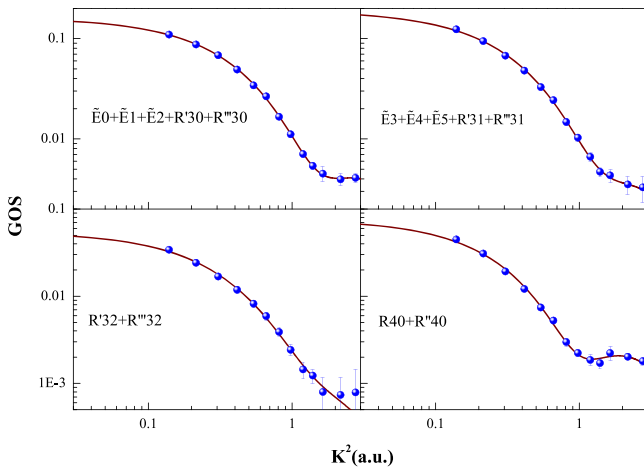


Figure 3. Present GOSs of the $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ excitations of the acetylene molecule. The dots are the present results, and the solid lines are their fitted curves.

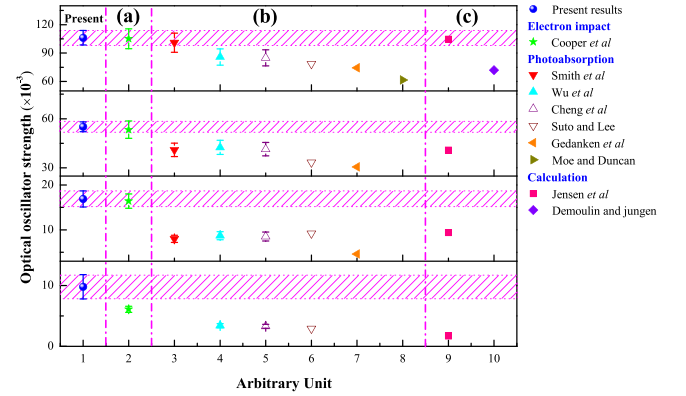


Figure 4. Present OOSs of the R30, R31, R32, and R33 excitations of acetylene along with the previously available ones from top to bottom.

our surprise, the discrepancies between the present OOSs and the photoabsorption ones of Wu et al. (2001), Cheng et al. (2011), Suto & Lee (1984), and Smith et al. (1991) gradually become larger and larger from the intense R30 transition to the weak R33 transition. This phenomenon for the R30–R33 excitations is distinctly different from the typical behavior of the line-saturation effect in which the discrepancies between the OOSs measured by the photoabsorption method and the true OOSs are larger and larger for the stronger and stronger transitions, such as the behavior of nitrogen (Liu et al. 2016). The rotational lines of the acetylene molecule seriously broaden and overlap due to the fast dissociation, causing the rotational structures of the R30–R33 transitions to disappear (Hu et al. 2008). Therefore, it is not likely that the more narrow widths of the higher vibronic states result in lower values of the OOSs measured by the photoabsorption method. Additionally, with the increasing of the ν_2' mode of the R30–R33 transitions, the continuum oscillator strength underlying the R30–R33 transitions becomes more significant, i.e., more comparable to the OOSs of the R30–R33 transitions for the present OOSs and the dipole (e, e) ones (Cooper et al. 1995). However, the contributions of the continuum oscillator strength underlying the R30–R33 transitions for the OOSs by the photoabsorption method are lower than those for the present OOSs and the dipole (e, e) ones (Cooper et al. 1995). So it is

Table 2
The OOSs of the Valence-shell Excitations of Acetylene

	R30	R31	R32	R33	$\tilde{E}0 + \tilde{E}1 + \tilde{E}2$ +R'30 + R''30	$\tilde{E}3 + \tilde{E}4 + \tilde{E}5$ +R'31 + R''31	R'32 + R''32	R40 + R''40
Present OOSs	106.2(7.7)	55.1(3.0)	16.9(1.8)	9.8(2.0)	161.7(8.2)	189.7(10.6)	54.7(5.5)	76.4(6.9)
Electron impact								
Cooper et al. (1995)	105.2(10.5)	53.3(5.3)	16.4(1.6)	6.1(0.5)	161.0(16.1)	185.5(18.6)	53.4(5.3)	76.0(7.6)
Photoabsorption								
Smith et al. (1991)	101.0(10.1)	41.0(4.1)	8.0(0.8)	...	...	...	...	...
Wu et al. (2001)	85.9(8.6)	42.5(4.3)	8.7(0.9)	3.4(0.4)	...	...	...	...
Cheng et al. (2011)	85.0(8.5)	41.4(4.1)	8.5(1.0)	3.3(0.4)	...	...	...	...
Suto & Lee (1984)	78.5	33.3	9.2	2.9	...	...	38.2	51.2
Gedanken & Schnepf (1976)	74.3	30.6	4.6	...	...	...	...	...
Moe & Duncan (1952)	61.6	...	...	...	...	...	...	22.9
Theoretical calculation								
Jensen et al. (1990)	104.6	40.8	9.4	1.7	...	...	...	...
Demoulin & Jungen (1974)	72.0	...	...	...	...	...	...	...

Note. The listed data are amplified by a factor of 10^3 . The data in parentheses represent the corresponding experimental uncertainties.

likely that the large differences between the OOSs of the R30–R33 transitions at high v_2' are caused by the differences in the measurement methods and/or analysis of this continuum oscillator strength.

As for the theoretical calculation, it is clear from Figure 4(c) that for the R30 transition the present OOSs matches the calculated value from Jensen et al. (1990), but are higher than the calculations of Demoulin & Jungen (1974), while for the R31, R32, and R33 transitions, the present OOSs are higher than the calculations of Jensen et al. (1990).

In addition, the OOSs of the $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ excitations of the acetylene molecule are also determined according to Equation (2), and are shown in Figure 5 and Table 2. It is clear from Figure 5 that the present OOSs of these excitations match the dipole (e, e) ones of Cooper et al. (1995) well. Meanwhile, the present results are higher than the early photoabsorption results of Suto & Lee (1984) and Moe & Duncan (1952) for the $R'32 + R''32$ and $R40 + R''40$ excitations, which may be due to the limitations of the technique at that time.

Recently, Kim (2001, 2007) developed the *BE*-scaling method to calculate the ICSs of the dipole-allowed excitations of atoms and molecules based on the scaled plane-wave Born models, and reliable ICSs for many atoms and molecules (Tanaka et al. 2016) have been determined by the *BE*-scaling method, such as He, H₂ and CO. As pointed out by Tanaka et al. (2016), the *BE*-scaling method has the advantage of producing reliable ICSs at low impact energies and bridges the large gap between low-energy and high-energy electron-scattering. The *BE*-scaled ICSs $\sigma_{BE}(E_0)$ can be written as

$$\sigma_{BE}(E_0) = \frac{E_0}{E_0 + B + E_n} \sigma_{\text{Born}}(E_0). \quad (3)$$

Here, B is the binding energy. $\sigma_{\text{Born}}(E_0)$ stands for the Born cross section at an incident electron energy of E_0 :

$$\sigma_{\text{Born}}(E_0) = \frac{\pi}{E_0 E_n} \int_{K_{\min}^2}^{K_{\max}^2} \frac{f(K, E_n)}{K^2} dK^2. \quad (4)$$

$K_{\max}^2$ and $K_{\min}^2$ represent the maximum and minimum squared momentum transfers, respectively.

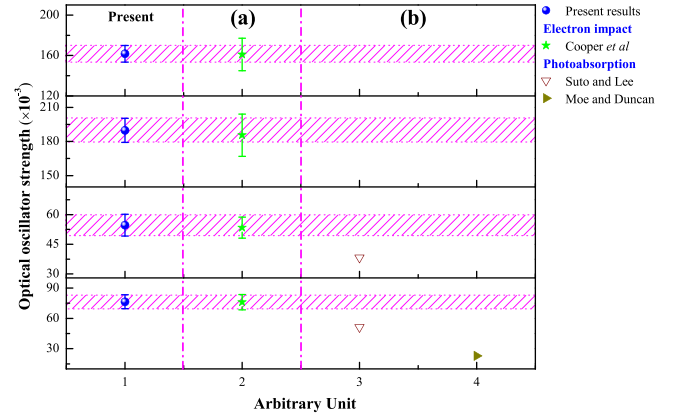


Figure 5. Present OOSs of the $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ excitations of acetylene along with the previously available ones from top to bottom.

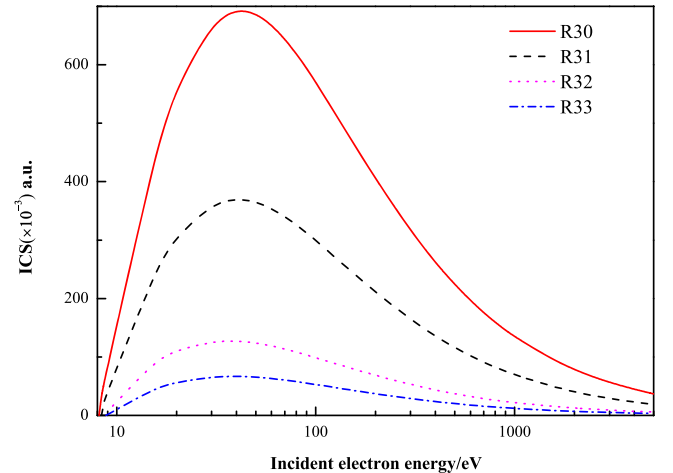


Figure 6. Present ICSs of the R30, R31, R32, and R33 excitations of acetylene at different electron impact energies.

Then, based on the present GOSs, the ICSs of the valence-shell excitations of acetylene are obtained from the threshold to 5000 eV with the aid of the *BE*-scaling method according to Equations (1)–(4), which are shown in Figures 6 and 7 and Table 3. Moreover, the ICSs of the valence-shell excitations of

Table 3
Present ICSs of Valence-shell Excitations of Acetylene from the *BE*-Scaling Method (in Atomic Units) at Different Electron Impact Energies

E_0 (eV)	R30	R31	R32	R33	$\tilde{E}0 + \tilde{E}1 + \tilde{E}2$ + $R'30 + R''30$	$\tilde{E}3 + \tilde{E}4 + \tilde{E}5$ + $R'31 + R''31$	$R'32 + R''32$	$R40 + R''40$
15	420.5	231.8	86.7	43.6	727.5	674.3	156.8	157.4
17.5	500.7	274.8	101.1	51.3	853.2	811.4	193.0	204.3
20	559.1	305.3	110.8	56.7	939.8	909.2	219.6	239.9
30	671.5	361.5	126.7	65.9	1087.2	1091.3	272.8	316.0
40	695.7	371.5	127.7	67.1	1102.5	1127.3	286.7	340.7
50	688.1	365.6	124.1	65.5	1075.5	1112.3	286.0	345.0
60	668.3	353.8	119.0	63.1	1034.2	1078.3	279.3	340.5
70	644.0	340.0	113.6	60.5	989.4	1037.7	270.3	331.9
80	618.8	326.0	108.4	57.8	945.1	995.8	260.5	321.8
90	594.0	312.4	103.4	55.3	903.0	955.0	250.7	311.1
100	570.4	299.6	98.8	52.9	863.6	916.2	241.2	300.5
150	473.3	247.4	80.6	43.5	707.2	757.9	201.4	254.1
200	404.7	211.0	68.3	36.9	599.9	646.7	172.8	219.5
300	316.1	164.3	52.7	28.6	464.2	503.8	135.5	173.5
400	261.4	135.6	43.3	23.6	381.6	415.9	112.3	144.4
500	224.0	116.0	36.9	20.1	325.7	355.9	96.3	124.3
600	196.7	101.8	32.3	17.6	285.2	312.2	84.7	109.5
700	175.8	90.9	28.8	15.7	254.3	278.9	75.7	98.1
800	159.3	82.3	26.0	14.2	229.9	252.5	68.6	89.1
900	145.8	75.3	23.8	13.0	210.1	231.0	62.9	81.7
1000	134.7	69.5	21.9	12.0	193.7	213.2	58.1	75.5
1500	98.4	50.7	15.9	8.7	140.9	155.5	42.5	55.4
2000	78.3	40.3	12.6	6.9	111.8	123.6	33.8	44.3
2500	65.5	33.7	10.5	5.8	93.2	103.2	28.3	37.1
3000	56.5	29.0	9.1	5.0	80.2	89.0	24.4	32.0
4000	44.6	22.9	7.1	3.9	63.2	70.2	19.3	25.3
5000	37.0	19.0	5.9	3.3	52.4	58.3	16.0	21.1

Note. The listed data are amplified by a factor of 10^3 .

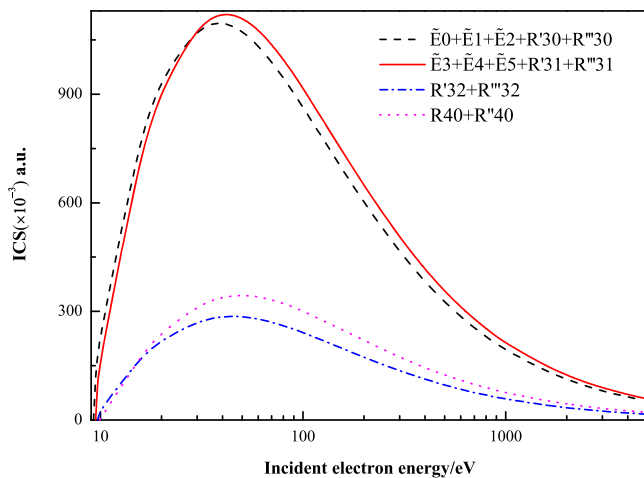


Figure 7. Present ICSs of the $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$, $\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ excitations of acetylene at different electron impact energies.

acetylene are obtained systematically for the first time. Unfortunately, there are no other theoretical calculations and experimental measurements for comparison, to the best of our knowledge, so further research on the ICSs of the valence-shell excitations of acetylene is greatly recommended.

4. Summary and Conclusions

In the present work, the GOSs of the valence-shell excitations of R30–R33, $\tilde{E}0 + \tilde{E}1 + \tilde{E}2 + R'30 + R''30$,

$\tilde{E}3 + \tilde{E}4 + \tilde{E}5 + R'31 + R''31$, $R'32 + R''32$, and $R40 + R''40$ of acetylene have been determined by the high-energy electron-scattering technique. Based on the present GOSs, the OOSs of the valence-shell excitations of acetylene have been obtained by extrapolating the GOSs to the limit of the squared momentum transfer $K^2 \rightarrow 0$. It is found that the OOSs for the R30–R33 excitations measured by the photoabsorption method violate the typical behavior of the line-saturation effect, possibly because of fast dissociation of acetylene and the effect of the continuum oscillator strength underlying the R30–R33 transitions. The present OOSs provide an independent cross-check on previous experimental and theoretical results, and can serve as benchmark data. Moreover, the ICSs of the valence-shell excitations of acetylene have been obtained systematically from the threshold to 5000 eV for the first time with the aid of the newly developed *BE*-scaling method. The present OOSs and ICSs of the valence-shell excitations of acetylene serve an important role in modeling the abundance of acetylene in the upper atmospheres of Jupiter, Saturn, Titan, Uranus, Neptune, and Pluto, and are crucial for improving these atmospheric models.

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